

Recent Advances in Science Support for Isolated Droplet Combustion Experiments

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INTRODUCTION

In a joint program involving Prof. F.A. Williams of the University of California, San Diego and Dr. V. Nayagam of the National Center for Microgravity Research, the combustion characteristics of isolated liquid fuel droplets of n-heptane, n-decane, methanol, methanol-water, ethanol and ethanol-water having initial diameters between about 1 mm and 6 mm continues to be investigated. The objectives of the work are to improve fundamental knowledge of droplet combustion dynamics for pure fuels and fuel-water mixtures through microgravity experiments and theoretical analyses. The Princeton contributions support the engineering design, data analysis, and data interpretation requirements for the study of initially single component, spherically symmetric, isolated droplet combustion studies through experiments and numerical modeling. UCSD contributions are described in a companion communication in this conference. The Princeton effort also addresses the analyses of Fiber Supported Droplet Combustion (FSDC) experiments conducted with the above fuels and collaborative work with others who are investigating droplet combustion in the presence of steady convection. A thorough interpretation of droplet burning behavior for n-heptane and n-decane over a relatively wide range of conditions also involves the influences of sooting on the combustion behavior, and this particular aspect on isolated burning of droplets is under consideration in a collaborative program underway with Drexel University (M.Y. Choi and collaborators). This collaboration is addressed in another communication at this conference.

The one-dimensional, time-dependent, numerical modeling approach that we have continued to evolve for analyzing isolated, quiescent droplet combustion data has been further applied to investigate several facets of isolated droplet burning of simple alcohols, n-heptane, and n-decane. Some of the new results are described below.

LIQUID DENSITY EFFECTS ON ETHANOL DROPLET COMBUSTION

In a recent paper, we quantitatively evaluated the effects of thermal expansion and solution density variations on liquid drop diameter over the burning history of ethanol and ethanol water droplets [1]. We treated the liquid mass and thermal transport via “effective” empirical transport corrections (as we previously have done), and additionally considered a radial convective liquid flow velocity component in the governing equations to assess the importance of variations in the local liquid-phase density.

We found that the effects of liquid phase density changes are primarily confined to the initial droplet heat-up period where an increase in droplet diameter due to thermal expansion results in large negative contributions to the observed rate of droplet diameter change. After the initial heat-up period is over, the contribution becomes much less important than that from the actual liquid gasification rate, becoming mildly competitive again near the condition of extinction. At extinction, the gasification rate ceases while an increase in liquid water content and subsequent cooling both result in droplet contraction. The observed difference in drop diameters between cases with and without consideration of liquid density changes is within about 6 %.

Since the effects associated with liquid density changes are confined to a very short initial period in the overall droplet gasification history, they can be essentially compensated for by shifting the gasification rate curve. In other words, when plotted against the “extent of burning” coordinate, $1 - (d/d_0)^2$, the gasification rate curves match within about 2 % during most of the burning history. The integrated total water mass fraction histories in the liquid phase agree well within the uncertainty with which this parameter can be determined experimentally.

The analyses show that the liquid phase density terms in the governing equations do not affect significantly the model results for ethanol droplet combustion. By ignoring these terms, the numerical stiffness of the computations can be significantly reduced. Once robust droplet burning is established, there is very little “memory” of the initial transient heat-up period (as long as the applied ignition energy does not overdrive the process) in the subsequent computational predictions. All microgravity droplet combustion experiments involve some asymmetry initially, due to ignition. However, these results support the assumption that experimental burning histories can still be compared with uni-dimensional model results by matching the parts of the curves subsequent to the initial heat up period. Nearly all investigators that have performed microgravity experiments in droptowers and on space platforms have employed this assumption. It should be stressed that results may be different for pure droplet vaporization, but certainly the terms in question can be neglected in the analysis of microgravity experiments in which relative gas phase and droplet velocities are small and one is interested in burning rate, flame structure and extinction in the robust phases of burning.

TWO-STAGE IGNITION OF n-HEPTANE DROPLETS

Several microgravity studies on the thermal ignition behavior of n-heptane droplets have appeared, one of the more recent being that of Schnaubelt et al.[2]. Data typically have been generated by exposing a droplet that was initially at room temperature to a high ambient temperature within a surrounding “oven”. Two-stage type ignition processes have been observed, with complex kinetics suggested as the principal source of the behavior. With the exception of the above work, numerical modeling of the experiments has not utilized reaction mechanisms that included low-temperature, intermediate-temperature, and high-temperature kinetics in significant detail. We used our numerical model with the kinetics of Peters et al. [3] to investigate the two-stage ignition character of an n-heptane droplet immersed in a hot oxidizing environment.

Figure 1 depicts the calculated thermal ignition and gasification rate as functions of time for a 0.7mm n-heptane droplet instantaneously immersed in air with different far-field gas temperatures from 600-950 K. At far-field temperatures higher than 950 K, a short period of droplet heating and gasification leads to flaming ignition and the establishment of a high temperature diffusion flame surrounding the droplet. The gasification rate of the droplet increases very rapidly due to heat conducted to the droplet surface. The vapor formed diffuses away from the surface into

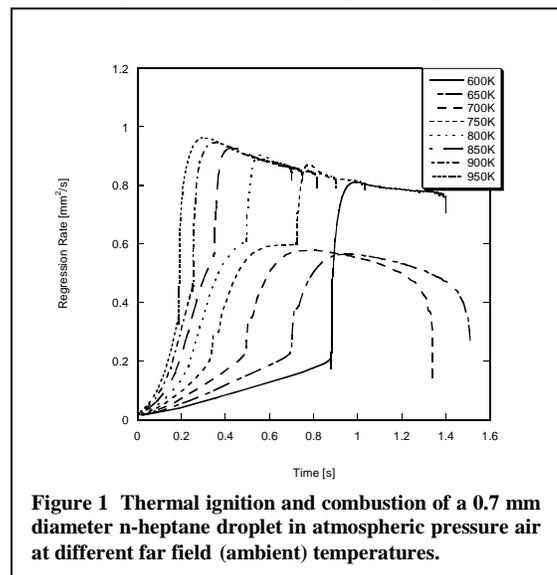


Figure 1 Thermal ignition and combustion of a 0.7 mm diameter n-heptane droplet in atmospheric pressure air at different far field (ambient) temperatures.

the surrounding hot gases and begins to react with oxygen, producing localized heating of the mixture. The localized chemical heat release leads to the occurrence of a flaming ignition. Little local heat release is needed to drive the local region into explosively fast, chain branched (high temperature) kinetic behavior within the fuel vapor surrounding the droplet (where oxygen is also present). The exact region where this occurs is a complex function of temperature, local equivalence ratio and time. The region of ignition leads to propagation of reaction through the remaining stratified pre-mixed layer of fuel species and oxidizer and a sharp increase in gasification rate due to the accompanying rapid heat release. This transitions into the typical diffusive flame structure observed to be surrounding a burning droplet. Subsequently, a burning rate above $0.8 \text{ mm}^2/\text{s}$ is achieved. This burning rate is consistent with the combustion of the same size n-heptane droplet and far-field temperature, but established by the ignition processes used to emulate spark ignition (as in our previous calculations).

For lower far-field ambient temperatures in air, the period of gasification prior to establishing a high temperature diffusion flame structure becomes longer. The droplet is consumed initially with a slower increase in gasification rate with time. As chemical heat release builds in the gas phase from the vaporized n-heptane diffusing into the surrounding hot oxidizer, the regression rate increases due to increases in the local gas temperatures near the drop surface. This characteristic persists at ambient temperatures between 950 K down to ones approaching 800 K. Note that the 800 K case shows an abrupt change in the gasification rate at about 0.35 seconds, a short time span over which the gasification rate increases very little with time, followed by a period in which the gasification rate again increases rapidly to that found for established diffusive burning. This behavior occurs because the portion of the fuel-vapor/air mixture with conditions that lie in the intermediate and high temperature kinetic regimes at higher ambient far field temperatures now partially lie within a temperature range characteristic of negative temperature coefficient (NTC) behavior and the chemical heat release rate available to modify the temperature profile is reduced. Sufficient heat release eventually exists to drive the region to temperatures characteristic of the high temperature regime (explosively fast chemistry), and the remaining system is driven to flaming ignition and a diffusion flame structure the same as that achieved for initially higher far field temperatures.

The same droplet in ambient air at temperatures from 800 K to approaching 600 K behave differently than those with either higher or lower far field temperature conditions. As the far field temperature drops, the characteristic period of the plateau region increases and the heat release that can occur is lessened to an extent that overall, none of the reacting environment can be driven into explosively fast chemical kinetic behavior before the droplet has been entirely consumed. As regions are driven to conditions within the parameter space characterized by NTC kinetic behavior, the destruction of n-heptane in those regions and heat release rate become very slow. Some the vaporized fuel in these regions is not consumed over the lifetime of the drop, even though it is mixed with oxidizer. Thus, although the droplet gasifies completely, a substantial fraction of the n-heptane vapor formed escapes to the ambient.

Interestingly, when the far-field temperature is reduced below 650K to 600 K, the slowing of the gasification rate disappears, and the system is driven to explosively fast kinetic behavior and the same diffusive flame structure found for the high temperature far field conditions again. In these cases, large regions of the reaction layer surrounding the droplet are at conditions characteristic of low temperature oxidation kinetics, and the accompanying heat release is so

rapid and large that conditions are driven through those characterizing NTC behavior and to explosively fast kinetic behavior.

A similar parametric study is shown in Fig. 2 for a larger 1.4 mm diameter n-heptane droplet over the same range of initial conditions. The size of the droplet affects the period of droplet heating, its gasification rate during the initial phases of gasification, the thickness of the layer of fuel-vapor/oxidizer/intermediate reaction species surrounding the drop, and its volume relative to the mass of liquid. In addition the time scale of relevance (gasification time of the drop) also changes. As a result the coupling with low, NTC, intermediate, and high temperature reaction kinetics lead to a different ignition and burning behavior. Now, no conditions are evidenced that eventually reach flaming combustion conditions. However, it is clear from inspection of these curves that, between 700 and 800K, there remains a period over which some of the regions surrounding the droplet exhibit NTC kinetic behavior, slowing the rate of gasification by reducing the rate of gas phase chemical heat addition.

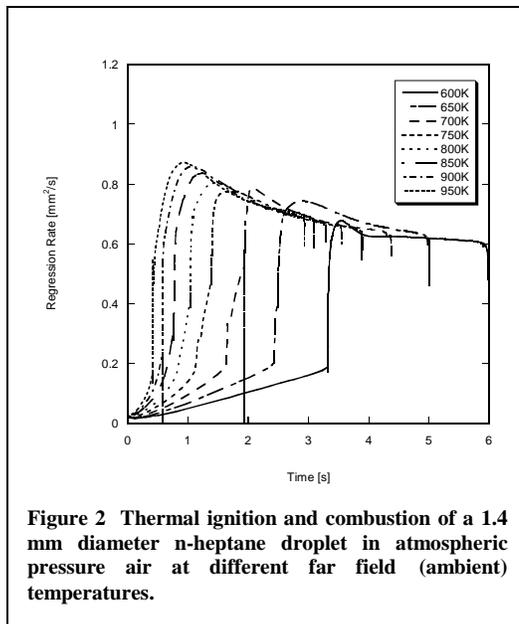


Figure 2 Thermal ignition and combustion of a 1.4 mm diameter n-heptane droplet in atmospheric pressure air at different far field (ambient) temperatures.

Further calculations are presently underway using a minimized mechanism [4] derived from the large detailed n-heptane oxidation mechanism published by Curran et al. [5].

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